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(*E*)-*N*′-[3-Methoxy-2-(2-nitrobenzyloxy)benzylidene]-isonicotinohydrazide

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Key indicators

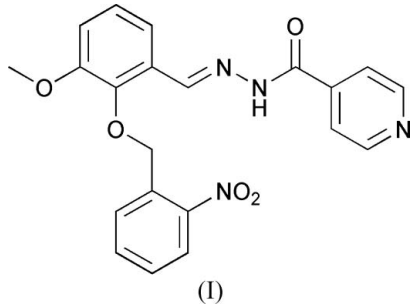
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.057
wR factor = 0.129
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{21}H_{18}N_4O_5$, crystallizes with two molecules in the asymmetric unit. The conformations of these non-planar molecules are simlilar. Intra- and intermolecular N—H···(O,N) hydrogen-bond systems and intermolecular C—H···O and C—H···N hydrogen bonds help to consolidate the crystal packing.

Comment

There has been steady growth of interest in the structure and reactivity of Schiff bases due to their potential biological activities, such as antibacterial and antitumor (Larson & Pecoraro, 1991; Santos *et al.*, 2001). Among the large number of such compounds, isonicotinohydrazide forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of these compounds, such as (*E*)-*N*′-[2-(4-chlorobenzyloxy)benzylidene]isonicotinohydrazide (Zhang *et al.*, 2006) and (*E*)-*N*′-[4-(2-chlorobenzyloxy)benzylidene]isonicotinohydrazide (Zhao *et al.*, 2006), have been reported. The title compound, (I) (Fig. 1), is another example of this family.



(I)

The asymmetric unit of (I) consists of two independent molecules, which are similar to each other. All the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). In molecule 1, the *o*-vanillin group (C7–C13/O2/O3) is planar, with an r.m.s. deviation, δ, from the mean plane of 0.0282 Å. It makes dihedral angles of 44.92 (10) and 85.36 (7)° with the pyridine ring (C1–C5/N1) and the nitrobenzene ring (C16–C21), respectively. In molecule 2, the *o*-vanillin group (C28–C34/O7/O8) is also planar, with δ = 0.0332 Å, and it makes dihedral angles of 61.98 (9) and 89.47 (7)° with the pyridine ring (C22–C26/N5) and the nitrobenzene ring (C37–C42), respectively.

Bifurcated N—H···(O,N) intra- and intermolecular hydrogen-bond systems are found in (I) (Table 1 and Fig. 2), which help to consolidate the crystal packing. The crystal structure of (I) also contains four weak intermolecular hydrogen bonds, two C—H···N and two C—H···O.

Experimental

An anhydrous ethanol solution (50 ml) of 2-(2-nitrobenzyloxy)-3-methoxybenzaldehyde (2.87 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of isonicotinohydrazide (1.37 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen, giving a yellow precipitate. The product was isolated and recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 82% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{21}H_{18}N_4O_5$
M_r = 406.39
Monoclinic, $P2_1/c$
a = 7.8965 (17) Å
b = 26.120 (6) Å
c = 20.139 (4) Å
β = 96.355 (4)°
V = 4128.3 (15) Å^3
Z = 8
D_x = 1.308 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, yellow
0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.989
23178 measured reflections
8411 independent reflections
3364 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.129
S = 1.01
8411 reflections
544 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0021 (2)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···O6	0.86	2.32	2.957 (3)	131
N2—H2*A*···N7	0.86	2.54	3.314 (3)	150
N6—H6···O1^{i}	0.86	2.34	2.894 (3)	123
N6—H6···N3^{i}	0.86	2.53	3.365 (3)	165
C25—H25···N3^{i}	0.93	2.55	3.382 (4)	150
C40—H40···O9^{i}	0.93	2.56	3.448 (4)	159
C32—H32···N5^{ii}	0.93	2.45	3.299 (4)	151
C14—H14*C*···O10^{ii}	0.96	2.54	3.445 (4)	157

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$.

The H atoms were included in calculated positions and refined using a riding model approximation. Constrained C—H and N—H bond lengths and isotropic U parameters: 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H; 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene C—H; 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl C—H; 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for imino N—H.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

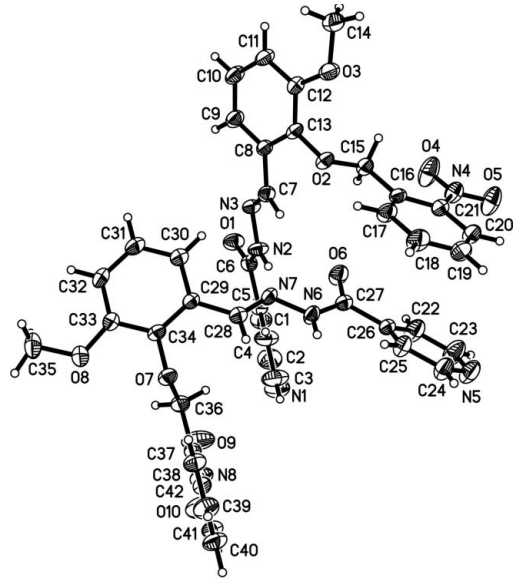


Figure 1
The asymmetric unit of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

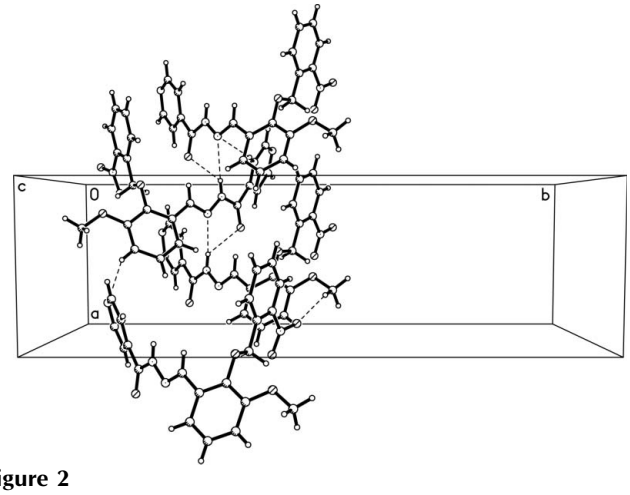


Figure 2
Partial packing diagram for (I), with hydrogen bonds drawn as dashed lines.

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